



Pergamon

Topology Vol. 35, No. 1, pp. 77–87, 1996
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 0040-9383/96 \$15.00 + 0.00

0040-9383(95)00002-X

TOPOLOGICAL INVARIANTS OF GRAPHS IN 3-SPACE

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(Received 15 October 1993; in revised form 30 November 1994)

1. INTRODUCTION

A graph G , in abstract terms, is a set of *vertices*, denoted by $V(G)$, together with a set of *edges*, denoted by $E(G)$, where just two vertices are associated with each edge at its *ends*. An edge is said to be *incident* to its ends, and the number of edges incident to a vertex v is called the *valence* at v . As usual, we shall regard graphs as 1-complexes whose 0- and 1-simplexes represent vertices and edges, respectively. Now, given a graph G , we consider its embeddings in 3-sphere S^3 . Two embeddings ξ and η of G are said to be *equivalent* if there exists an orientation preserving homeomorphism ζ of S^3 such that $\xi = \zeta \circ \eta$. To distinguish embeddings of G under this equivalence relation, we often need some *invariants*. A few examples of such invariants can be found in [2, 6–8].

In this article, we introduce new invariants of *arbitrary* graphs in S^3 which correspond to *Yamada polynomials* [7, 8] for graphs with constant valence 3. They are definitely computable, and powerful enough to detect some delicate differences of embeddings peculiar to graphs. To obtain such invariants, we start with *diagrams* which are images of embedded graphs under a projection $S^3 \rightarrow S^2$ whose singularities are a finite number of double points of edges equipped with over-under information. Note that we can definitely recover original embeddings from their diagrams. It is well-known that 2 diagrams represent equivalent embeddings of a graph if and only if they are related by a finite sequence of *Reidemeister moves* [7, 8] depicted in Fig. 1. Thus, to obtain an invariant of embedded graphs, we associate a quantity to each diagram which is invariant under Reidemeister moves.

We first introduce *linear skeins* [4] of planar surfaces in Section 2 to describe certain vector spaces in Section 3 which are associated to vertices of graphs. We then define our invariants, and present some properties in Section 4. Section 5 provides another description of the invariants, which will be more convenient for actual calculations. A few examples are also exhibited in Section 6, which tell us that our invariants are highly nontrivial.

2. LINEAR SKEINS

Let F be a compact, connected, two-dimensional submanifold of S^2 . A *diagram* on F is, here, immersed circles and arcs joining specified points on ∂F whose singular set consists of a finite number of double points equipped with over-under information. We do not distinguish two diagrams which are transformed into each other by isotopy of F relative to ∂F .

Definition (Lickorish [4]). Let A be a unit complex number. The *linear skein* $\mathcal{S}(F)$ of F is a complex vector space of linear sums of diagrams on F quotiented by relations

$$D \cup \bigcirc = -(A^2 + A^{-2}) \cdot D$$
$$\nearrow = A \frown + A^{-1} ($$

where \bigcirc stands for the boundary of a disk in F .

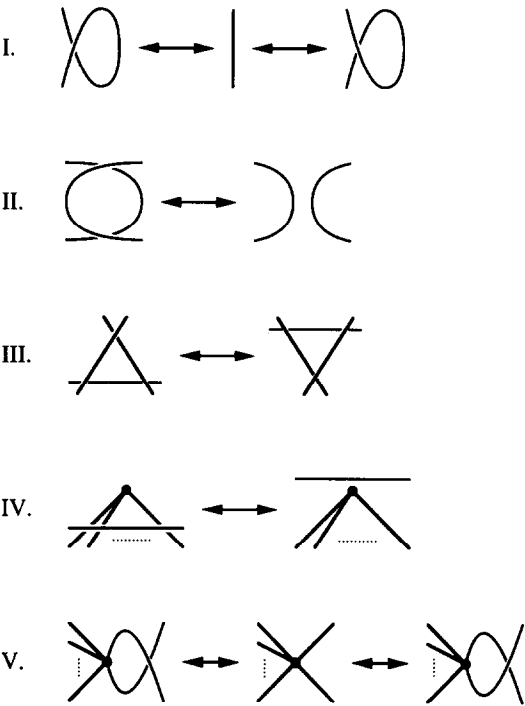


Fig. 1.

From the definition, as in the case of Kauffman’s bracket [1], two diagrams related by Reidemeister moves II, III define the same element of $\mathcal{S}(F)$. We begin with a fundamental example.

PROPOSITION 2.1 (Lickorish [4]). *If $D \in \mathcal{S}(S^2)$, then*

$$D = \langle D \rangle \cdot \emptyset,$$

where $\langle \cdot \rangle$ denotes Kauffman’s bracket with $\langle \bigcirc \rangle = -A^2 - A^{-2}$. Thus, $\mathcal{S}(S^2)$ is identified with \mathbb{C} .

In what follows, D_l denotes an oriented disk with $l \in 2\mathbb{Z}$ specified points on its boundary. Furthermore, for a partition $l = l_1 + \cdots + l_n$, $l_i > 0$, $D_{l_1} + \cdots + D_{l_n}$ denotes D_l equipped with disjoint n arcs on ∂D_l which cover l_1, \dots, l_n points in order with respect to the orientation of ∂D_l .

We now study $\mathcal{S}(D_{l+i})$, and define an important element f_l of $\mathcal{S}(D_{l+i})$ which is often abbreviated as in Fig. 2. We distinguish two arcs on ∂D_{l+i} as *upper* and *lower* ones. Then, for $\alpha, \beta \in \mathcal{S}(D_{l+i})$, define a product $\alpha\beta \in \mathcal{S}(D_{l+i})$ by gluing the lower arc of α and the upper arc of β , which makes $\mathcal{S}(D_{l+i})$ the l th Temperley–Lieb algebra. Let $f_1 \in \mathcal{S}(D_{1+1})$ be a single strand. Then, $f_l \in \mathcal{S}(D_{l+i})$ is inductively defined by Fig. 3, where

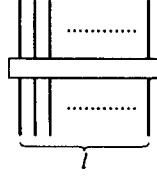


Fig. 2.

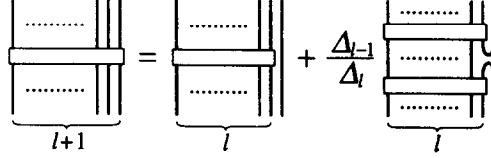


Fig. 3.

$$\Delta_m = (-1)^m \frac{A^{2(m+1)} - A^{-2(m+1)}}{A^2 - A^{-2}} \in \mathbf{R}.$$

Note that $f_l \in \mathcal{S}(D_{l+l})$ is defined only if

$$\Delta_1 \Delta_2 \cdots \Delta_{l-2} \neq 0.$$

This f_l has several interesting properties [4], which are pictorially presented in Fig. 4.

3. VECTOR SPACES

Consider diagrams in $D_{l_1+\dots+l_n}$ surrounded by f_{l_1}, \dots, f_{l_n} . Such diagrams form a subspace $\mathcal{H}_{l_1+\dots+l_n}$ of $\mathcal{S}(D_{l_1+\dots+l_n})$ which is nonempty if and only if each l_i does not exceed half of $l = l_1 + \dots + l_n$. In this section, we prove $\mathcal{H}_{l_1+\dots+l_n}$ has a positive definite Hermitian form θ , and explicitly give an orthonormal basis with respect to θ . From now on, we choose A so that

$$(-1)^m \Delta_m = \frac{A^{2(m+1)} - A^{-2(m+1)}}{A^2 - A^{-2}} > 0$$

for each m up to the half of l .

Let $-D_{l_1+\dots+l_n}$ denote $D_{l_1+\dots+l_n}$ with the opposite orientation. Note that the orientation reversing map

$$D_{l_1+\dots+l_n} \rightarrow -D_{l_1+\dots+l_n}$$

induces an isomorphism

$$*: \mathcal{H}_{l_1+l_2+\dots+l_n} \rightarrow \mathcal{H}_{l_n+\dots+l_2+l_1}$$

which takes complex conjugate for coefficients and mirror images for diagrams. By gluing $D_{l_1+\dots+l_n}$ and $-D_{l_1+\dots+l_n}$ at their boundary, we have an S^2 with n arcs on its equator, which defines a map

$$\mathcal{H}_{l_1+\dots+l_n} \times \mathcal{H}_{l_1+\dots+l_n} \rightarrow \mathcal{H}_{l_1+\dots+l_n} \times \mathcal{H}_{l_n+\dots+l_1} \rightarrow \mathcal{S}(S^2) \cong \mathbf{C}.$$

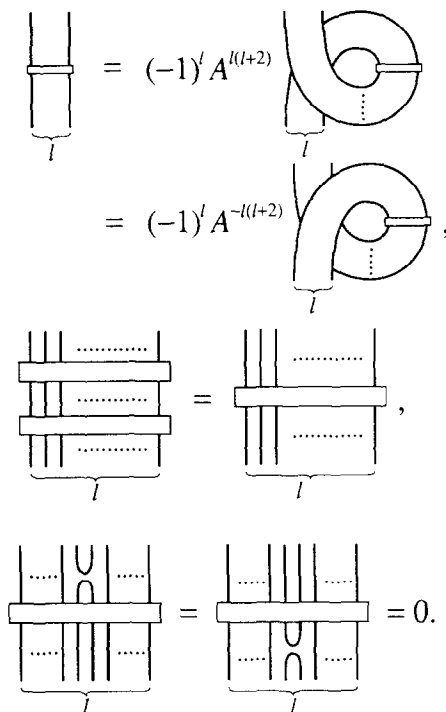


Fig. 4.

Multiplying this map by $\sqrt{-1}^l$, we obtain a Hermitian form

$$\theta: \mathcal{H}_{l_1 + \dots + l_n} \times \mathcal{H}_{l_1 + \dots + l_n} \rightarrow \mathbf{C}.$$

On the other hand, we define $\sigma_i^{\pm 1}: \mathcal{H}_{l_1 + \dots + l_i + l_{i+1} + \dots + l_n} \rightarrow \mathcal{H}_{l_1 + \dots + l_{i+1} + l_i + \dots + l_n}$ by Fig. 5.

PROPOSITION 3.1. $\sigma_i^{\pm 1}$ is unitary with respect to θ , that is,

$$\theta(\sigma_i^{\pm 1}(u), \sigma_i^{\pm 1}(v)) = \theta(u, v)$$

for any $u, v \in \mathcal{H}_{l_1 + \dots + l_n}$.

Proof. See Fig. 6. □

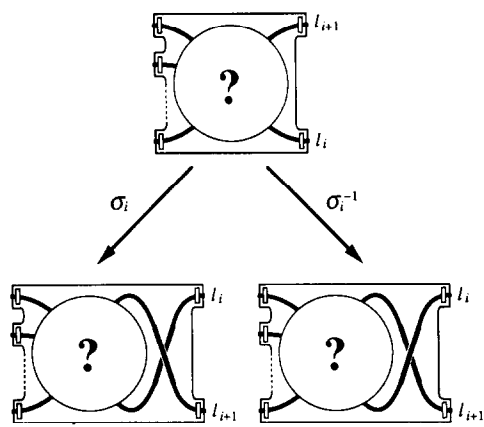
Thus, for any orthonormal bases of $\mathcal{H}_{l_1 + \dots + l_i + l_{i+1} + \dots + l_n}$ and $\mathcal{H}_{l_1 + \dots + l_{i+1} + l_i + \dots + l_n}$ with respect to θ , if they exist, $\sigma_i^{\pm 1}$ are represented by unitary matrices, which will play a key role to define invariants. Fortunately, a nice candidate is given in [3].

Definition. A triple (a, b, c) of non-negative integers is said to be *admissible* if

$$\begin{aligned} |a - b| &\leq c \leq a + b \\ a + b + c &\in 2\mathbf{Z}. \end{aligned}$$

In what follows, for admissible (a, b, c) , we use an abbreviation shown in Fig. 7 to describe a vector of \mathcal{H}_{a+b+c} where $x + y = a$, $y + z = b$ and $z + x = c$, and put

$$\Delta_{a,b,c} = \frac{\Delta_{x+y+z}! \Delta_{x-1}! \Delta_{y-1}! \Delta_{z-1}!}{\Delta_{y+z-1}! \Delta_{z+x-1}! \Delta_{x+y-1}!}$$



Here,

$$\begin{array}{c} \diagup \diagdown \\ a \quad b \end{array} = \begin{array}{c} \diagup \diagdown \\ a \quad b \end{array}$$

Fig. 5.

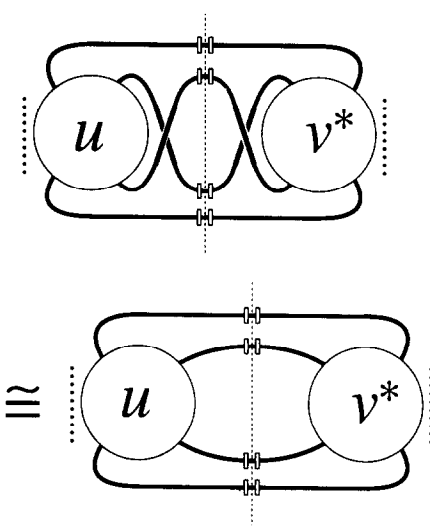


Fig. 6.

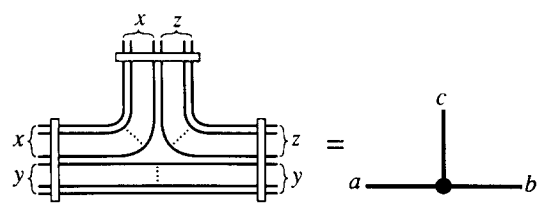


Fig. 7.

where $\Delta_m! = \Delta_m \Delta_{m-1} \cdots \Delta_0$ and $\Delta_{-1}! = 1$. Note that $\sqrt{-1}^{a+b+c} \Delta_{a,b,c}$ is positive real if $a + b + c \leq l$.

Let $\hat{u}(j_1, \dots, j_{n-3})$ denote a vector of $\mathcal{H}_{l_1+\dots+l_n}$ depicted in Fig. 8, where $(l_1, l_2, j_1), (j_1, j_2, l_3), \dots, (j_{n-3}, l_{n-1}, l_n)$ are admissible. By the identity [4] shown in Fig. 9, we have

$$\theta(\hat{u}(j_1, \dots, j_{n-3}), \hat{u}(j_1, \dots, j_{n-3})) = \sqrt{-1}^l \frac{\Delta_{l_1, l_2, j_1} \Delta_{j_1, j_2, l_3} \cdots \Delta_{j_{n-3}, l_{n-1}, l_n}}{\Delta_{j_1} \Delta_{j_2} \cdots \Delta_{j_{n-3}}}$$

which is *positive real* in our setting.

Let $\mathcal{B}_{l_1+\dots+l_n}$ denote the set of vectors

$$u(j_1, \dots, j_{n-3}) = \frac{\hat{u}(j_1, \dots, j_{n-3})}{\sqrt{\theta(\hat{u}(j_1, \dots, j_{n-3}), \hat{u}(j_1, \dots, j_{n-3}))}}$$

where j_1, \dots, j_{n-3} varies so that $(l_1, l_2, j_1), (j_1, j_2, l_3), \dots, (j_{n-3}, l_{n-1}, l_n)$ are admissible.

PROPOSITION 3.2. $\mathcal{B}_{l_1+\dots+l_n}$ is an orthonormal basis of $\mathcal{H}_{l_1+\dots+l_n}$.

Proof. By the argument in [3, Section 3], we can see that $\mathcal{H}_{l_1+\dots+l_n}$ is spanned by the above vectors. The orthonormality with respect to θ follows from the identity in Fig. 9 and the definition of $\mathcal{B}_{l_1+\dots+l_n}$, which immediately proves the independence. \square

4. INVARIANTS

Let G be an abstract graph. A *weight* ω of G is a map

$$\omega: E(G) \rightarrow \{0, 1, 2, 3, \dots\}.$$

Let v_1, v_2, \dots, v_r be vertices of G , $e_{i,1}, e_{i,2}, \dots, e_{i,n_i}$ the edges incident to v_i , and $l(i, 1), l(i, 2), \dots, l(i, n_i)$ weights on these n_i edges. A weight ω of G is said to be *admissible* if

$$2l(i, j) \leq \sum_{k=1}^{n_i} l(i, k) \in 2\mathbb{Z}$$

for each $1 \leq i \leq r$ and each $1 \leq j \leq n_i$.

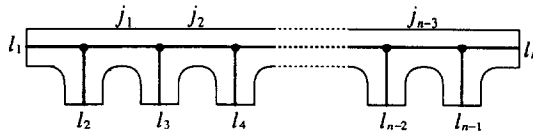


Fig. 8.

$$\begin{array}{c} a \\ | \\ \circ \\ | \\ b \quad \circ \quad c \\ | \\ a' \end{array} = \delta_{a,a'} \frac{\Delta_{a,b,c}}{\Delta_a} \quad \left| \begin{array}{c} a \\ | \\ a' \end{array} \right.$$

Fig. 9.

Now, consider an embedding $\xi: G \rightarrow S^3$ and a diagram D of $\xi(G)$ on S^2 , where the images of vertices and edges on S^2 are also denoted by the same symbols. By renumbering, for each i , we suppose $e_{i,1}, e_{i,2}, \dots, e_{i,n_i}$ are arranged in the counterclockwise direction on S^2 around v_i , and put $\mathcal{H}_i = \mathcal{H}_{l(i,1)+\dots+l(i,n_i)}$ for simplicity. For any $u_i \in \mathcal{H}_i$, we define

$$\langle u_1, u_2, \dots, u_r \rangle_{D,\omega} \in \mathcal{S}(S^2)$$

by replacing a neighborhood of each vertex, say v_i , with u_i and each edge, say $e_{i,j}$, with $l(i,j)$ parallel curves, where each double point is replaced as in Fig. 5. Thus, we have a multilinear form

$$\underbrace{\langle \dots \rangle}_{r, \omega}: \mathcal{H}_1 \times \dots \times \mathcal{H}_r \rightarrow \mathbb{C}.$$

From the property of Kauffman's bracket [1], the following is obvious.

PROPOSITION 4.1. *If D and D' are diagrams of $\xi(G)$ related by Reidemeister moves II, III, IV,*

$$\langle \dots \rangle_{D,\omega} = \langle \dots \rangle_{D',\omega}.$$

By the first identity in Fig. 4, we also have the following.

PROPOSITION 4.2. *If D and D' are diagrams of $\xi(G)$ related by a Reidemeister move I,*

$$|\langle u_1, \dots, u_r \rangle_{D,\omega}| = |\langle u_1, \dots, u_r \rangle_{D',\omega}|$$

for any $u_i \in \mathcal{H}_i$.

Let D and D' be diagrams related by a Reidemeister move V. We can suppose

$$\langle \dots \rangle_{D,\omega}: \mathcal{H}_1 \times \dots \times \mathcal{H}_{l(i,1)+\dots+l(i,j)+l(i,j+1)+\dots+l(i,n_i)} \times \dots \times \mathcal{H}_r \rightarrow \mathbb{C}$$

and

$$\langle \dots \rangle_{D',\omega}: \mathcal{H}_1 \times \dots \times \mathcal{H}_{l(i,1)+\dots+l(i,j+1)+l(i,j)+\dots+l(i,n_i)} \times \dots \times \mathcal{H}_r \rightarrow \mathbb{C}.$$

Let $\mathcal{B}, \mathcal{B}'$ be orthonormal bases of

$$\mathcal{H}_{l(i,1)+\dots+l(i,j)+l(i,j+1)+\dots+l(i,n_i)}, \quad \mathcal{H}_{l(i,1)+\dots+l(i,j+1)+l(i,j)+\dots+l(i,n_i)}$$

respectively. Then, by Proposition 3.1, we have the following.

PROPOSITION 4.3. *For any $u_k \in \mathcal{H}_k$, $k \neq i$,*

$$\sum_{u \in \mathcal{B}} |\langle u_1, \dots, u_{i-1}, u, u_{i+1}, \dots, u_r \rangle_{D,\omega}|^2 = \sum_{u \in \mathcal{B}'} |\langle u_1, \dots, u_{i-1}, u, u_{i+1}, \dots, u_r \rangle_{D',\omega}|^2.$$

Let \mathcal{B}_i be an orthonormal basis of \mathcal{H}_i for each $1 \leq i \leq r$. Define

$$Z(\xi, \omega) = \sum_{(u_1, \dots, u_r) \in \mathcal{B}_1 \times \dots \times \mathcal{B}_r} |\langle u_1, \dots, u_r \rangle_{D,\omega}|^2.$$

Note that $Z(\xi, \omega)$ does not depend on the choice of \mathcal{B}_i because two orthonormal bases are related by a unitary matrix. By Propositions 4.1–4.3, $Z(\xi, \omega)$ does not depend on the choice of diagram D , and so we obtain an invariant of $\xi: G \rightarrow S^3$ for each weight ω . Note also that $Z(\xi, \omega)$ is expressed as a *rational function* of A whose dominator depends only on (G, ω) . Thus, our invariants are essentially *polynomials* after suitable normalization.

Obvious identities derived from the definition are summarized here without proof. Unfortunately, our invariants cannot distinguish a graph in S^3 from its mirror image.

PROPOSITION 4.4. *If two embeddings ξ and $\xi^!$ of G are related by a reflection of S^3 , then $Z(\xi, \omega) = Z(\xi^!, \omega)$ for any weight ω .*

Let e be an edge of G .

PROPOSITION 4.5. *Let G' be G with a vertex added on e . An embedding ξ of G with an admissible weight ω induces an embedding ξ' of G' with an admissible weight ω' , and we have*

$$Z(\xi', \omega') = \Delta_{\omega(e)}^{-1} Z(\xi, \omega).$$

PROPOSITION 4.6. *Let G' be G with e identified to a vertex. An admissible weight ω' of G' specifies a set $\Omega(G, \omega')$ of admissible weights of G which are identical with ω' on $E(G) - e$. Let ξ be an embedding of G and ξ' an embedding of G' obtained from ξ by identifying $\xi(e)$ to a vertex. Then, we have*

$$Z(\xi', \omega') = \sum_{\omega \in \Omega(G, \omega')} \Delta_{\omega(e)} Z(\xi, \omega).$$

Let $S^3 = B_+ \cup B_-$ be a decomposition of S^3 into 3-balls B_\pm , and let $S^2 = \partial B_\pm$. We suppose that an embedding ξ of G satisfies $B_\pm \cap \xi(G) \neq \emptyset$, and that ω is an admissible weight of G .

PROPOSITION 4.7. *If $S^2 \cap \xi(G) = \emptyset$, then G is a disjoint union of subgraphs G_\pm , and*

$$Z(\xi, \omega) = Z(\xi|_{G_+}, \omega|_{G_+}) Z(\xi|_{G_-}, \omega|_{G_-}).$$

If $S^2 \cap \xi(G)$ is a midpoint of edge e , $Z(\xi, \omega) = 0$ because of the third identity in Fig. 4. Combining this with Proposition 4.7, we have the following.

PROPOSITION 4.8. *If $S^2 \cap \xi(G)$ is a midpoint of e , $G - e$ is a disjoint union of subgraphs G_\pm , and*

$$Z(\xi, \omega) = \begin{cases} 0 & \text{if } \omega(e) \neq 0 \\ Z(\xi|_{G_+}, \omega|_{G_+}) Z(\xi|_{G_-}, \omega|_{G_-}) & \text{if } \omega(e) = 0. \end{cases}$$

By Propositions 4.6 and 4.8, we have the following.

PROPOSITION 4.9. *If $S^2 \cap \xi(G)$ is a vertex v , G decomposes into 2 subgraphs G_\pm with $G_+ \cap G_- = v$, and*

$$Z(\xi, \omega) = Z(\xi|_{G_+}, \omega|_{G_+}) Z(\xi|_{G_-}, \omega|_{G_-}).$$

5. ANOTHER DESCRIPTION OF INVARIANTS

Let G be a graph with an admissible weight ω , and ξ an embedding of G in S^3 as above. Take a diagram D of $\xi(G)$. Then, we *blow up* each vertex of D , whose valence is greater than 3, to a trivalent tree as shown in Fig. 10. The resultant diagram is denoted by \hat{D} which is considered as a diagram of a trivalent graph \hat{G} embedded in S^3 .

Let $\Omega(\hat{G}, \omega)$ be the set of admissible weights of \hat{G} which agree with ω on $E(G) \subset E(\hat{G})$. For $\psi \in \Omega(\hat{G}, \omega)$ and $v \in V(\hat{G})$, put $\|v\|_\psi = \Delta_{a,b,c}$ where a, b, c are weights on three edges incident

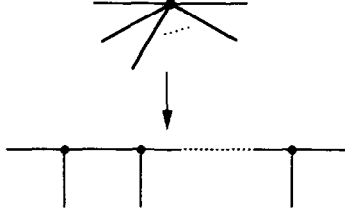


Fig. 10.

to v , and define

$$\|\psi\| = \frac{\prod_{e \in E(\hat{G}) - E(G)} \Delta_{\psi(e)}}{\prod_{v \in V(\hat{G})} \|v\|_{\psi}}.$$

Furthermore, according to \hat{D} and ψ , we define $\psi\hat{D} \in \mathcal{S}(S^2)$ by replacing each vertex and each edge of \hat{D} with parallel curves as before. Then, from the definition of Section 4, we have the following.

PROPOSITION 5.1.

$$Z(\xi, \omega) = \sum_{\psi \in \Omega(\hat{G}, \omega)} \|\psi\| \langle \psi\hat{D} \rangle \langle \psi\hat{D}^! \rangle,$$

where $D^!$ stands for the mirror image of D .

To present examples in the following section, we shall use this definition of invariants.

6. EXAMPLES

In this section, we calculate our invariant for two embedded graphs, which shows its nontriviality and effectiveness. Put $\Delta = -A^2 - A^{-2}$. Note that $\Delta_1 = \Delta$, $\Delta_2 = \Delta^2 - 1$ and the identity in Fig. 11.

Consider an embedding ξ of a *bouquet* determined by a diagram D in Fig. 12. To obtain a diagram \hat{D} of a trivalent graph \hat{G} , blow up the vertex of D as in Fig. 13. For the constant weight $\omega \equiv 1$, $\Omega(\hat{G}, \omega)$ consists of ψ_0 and ψ_2 which take the weights 0 and 2 on the new edge respectively. A calculation shows

$$\|\psi_0\| = \frac{1}{\Delta^2}, \quad \|\psi_2\| = \frac{1}{\Delta^2 - 1}.$$

Furthermore,

$$\langle \psi_0\hat{D} \rangle = \Delta^2$$

$$\langle \psi_2\hat{D} \rangle = \Delta(A^7 - A^3 - A^{-5})(A^{-7} - A^{-3} - A^5) - \Delta^{-1}\Delta^2.$$

Thus, we have

$$Z(\xi, \omega) = 1 + 2(t + t^{-1}) - (t^2 + t^{-2}) - (t^3 + t^{-3}) - (t^5 + t^{-5}) + (t^6 + t^{-6})$$

with $t = A^4$. Since the planar embedding of the bouquet with constant weight one has the value 1, ξ is not planar.

We next consider an embedding η of a θ_4 -curve [5] determined by a diagram D in Fig. 14. To obtain a diagram \hat{D} of a trivalent graph \hat{G} , blow up two vertices of D as shown in Fig. 15. For $\omega \equiv 1$, $\Omega(\hat{G}, \omega)$ consists of ψ_{00} , ψ_{02} , ψ_{20} and ψ_{22} which take the weights (0, 0),

$$\text{Bar on lines} = \text{Two lines} - \Delta^{-1} \text{Crossing}$$

Fig. 11.

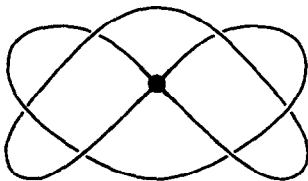


Fig. 12.

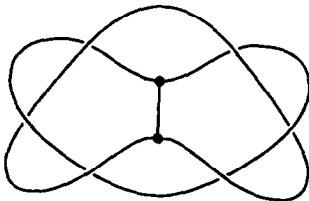


Fig. 13.

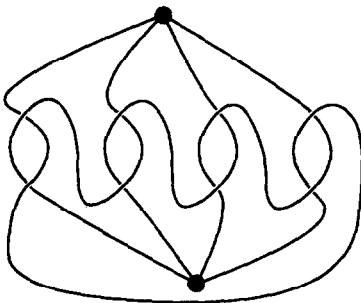


Fig. 14.

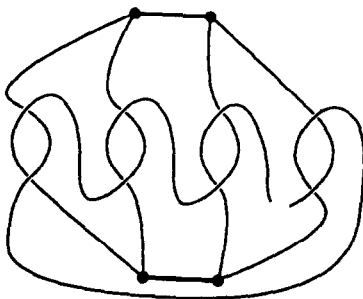


Fig. 15.

$(0, 2)$, $(2, 0)$ and $(2, 2)$ on new edges respectively. A calculation shows

$$\|\psi_{00}\| = \frac{1}{\Delta^4}, \quad \|\psi_{02}\| = \|\psi_{20}\| = \frac{1}{\Delta^2(\Delta^2 - 1)}, \quad \|\psi_{22}\| = \frac{1}{(\Delta^2 - 1)^2}.$$

Furthermore,

$$\begin{aligned} \langle \psi_{00} \hat{D} \rangle &= P \\ \langle \psi_{02} \hat{D} \rangle &= \langle \psi_{20} \hat{D} \rangle = Q - \Delta^{-1}P \\ \langle \psi_{22} \hat{D} \rangle &= P - 2\Delta^{-1}Q + \Delta^{-2}P \end{aligned}$$

where

$$\begin{aligned} P &= (-A^3)^{-8}(A^8 + 2A^{16} - 2A^{20} + A^{24} - 2A^{28} + A^{32})\Delta \\ Q &= (-A^{-18} + A^{-14} - 3A^{-10} + 2A^{-6} - 2A^{-2} + 2A^2 - A^6)\Delta. \end{aligned}$$

Thus, we have

$$Z(\eta, \omega) = 102 - 86(t + t^{-1}) + 56(t^2 + t^{-2}) - 26(t^3 + t^{-3}) + 6(t^4 + t^{-4}).$$

Since the planar embedding of a θ_4 -curve with constant weight one has the value 2, η is not planar.

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